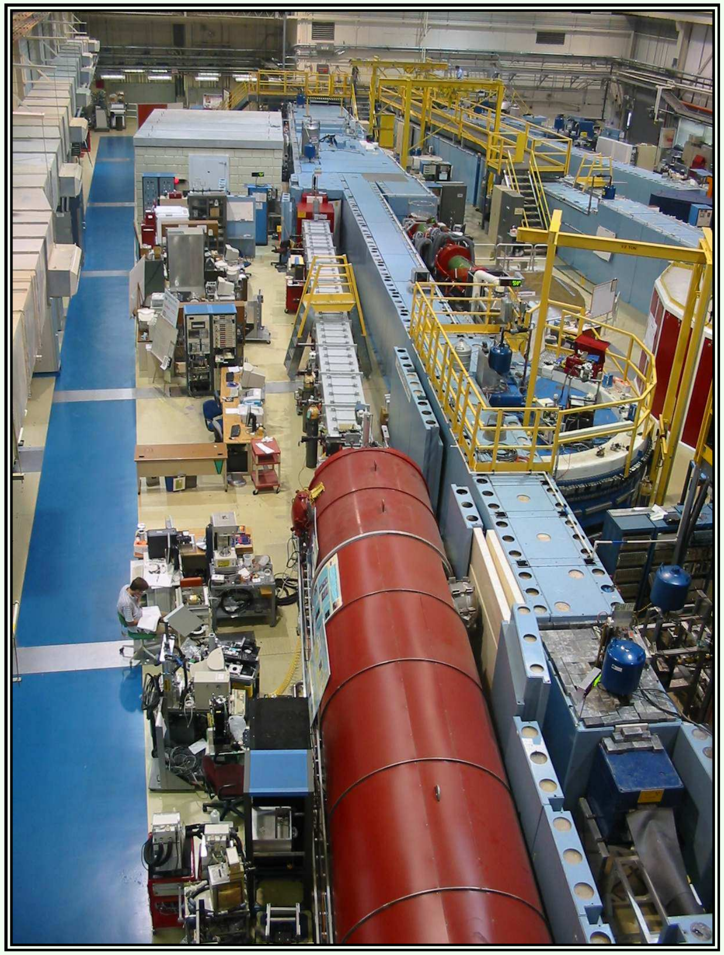
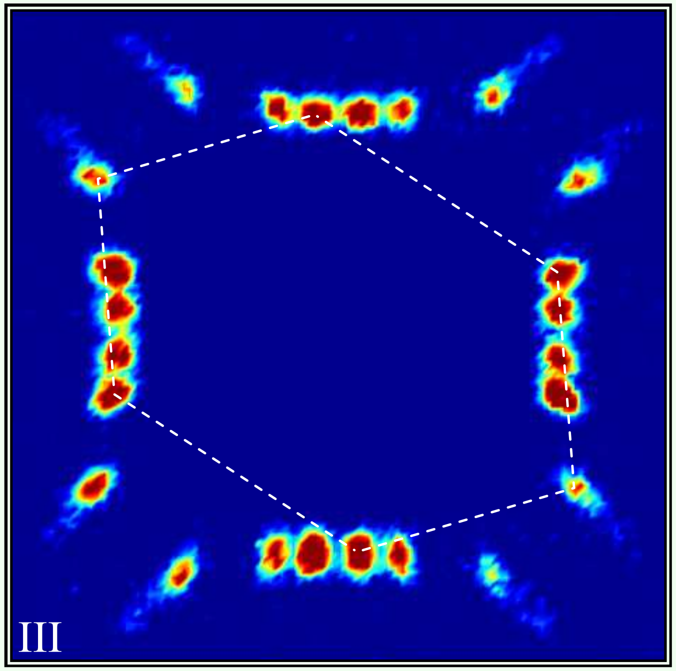
Magnetic SANS Theory

NCNR SANS Tutorial, February 2009

Mark Laver

NIST Center for Neutron Research, Gaithersburg, United States



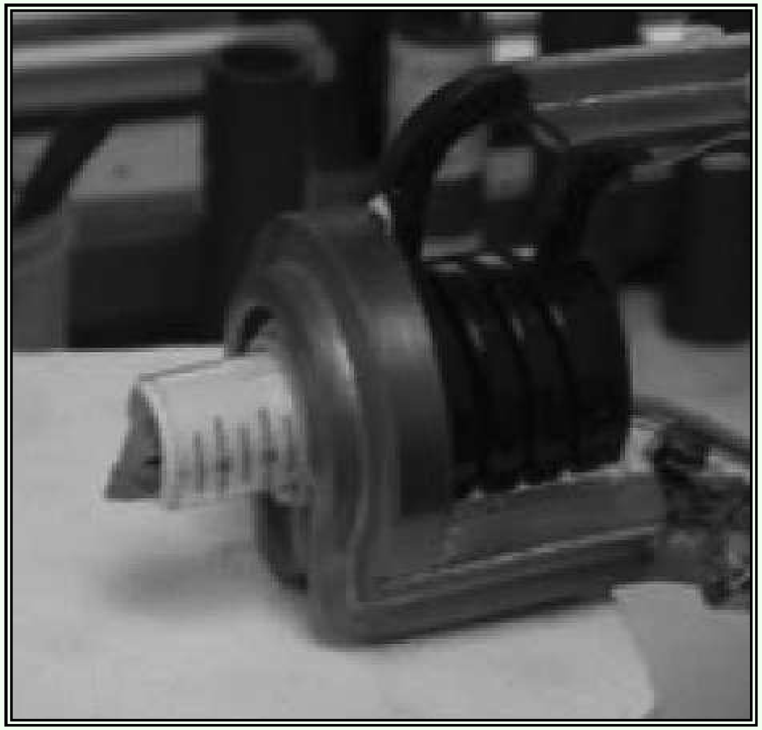


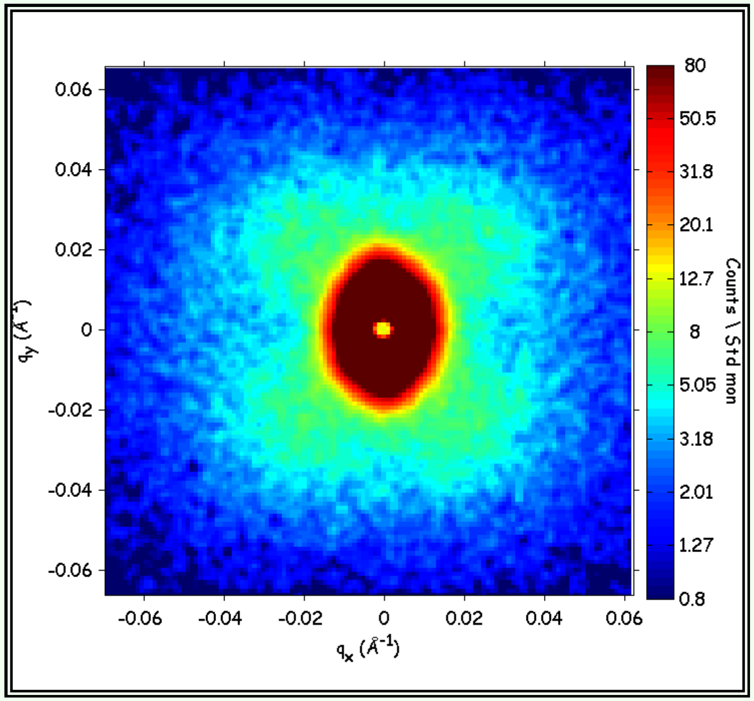
Flux line lattices in superconductors, skyrmion lattices

Magnetic nanoparticles

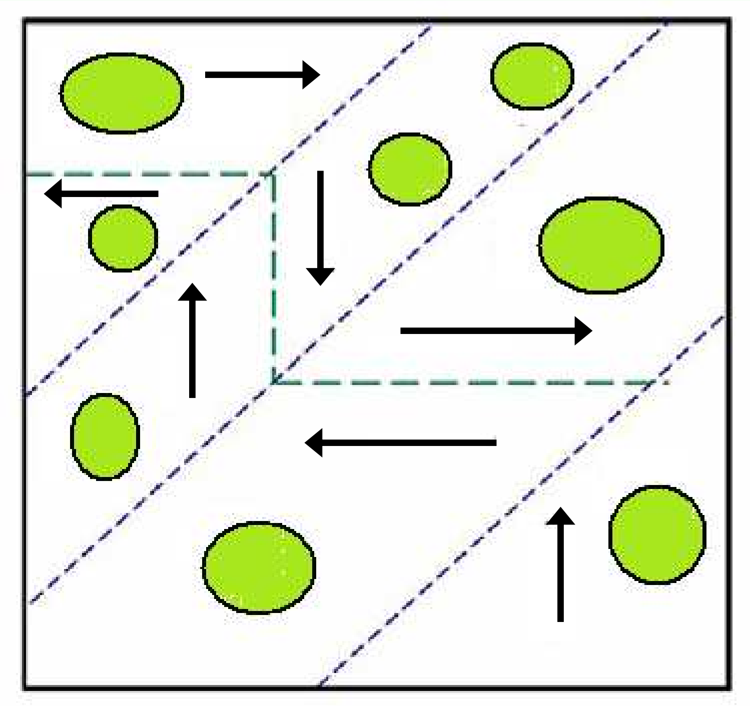
Films and nano-structured, engineered samples

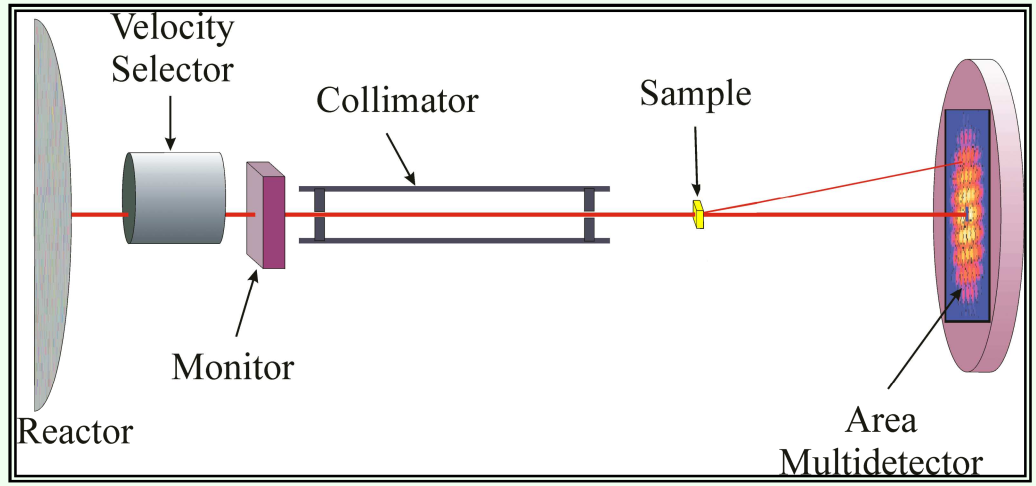
Phase separated systems, nanocrystalline materials



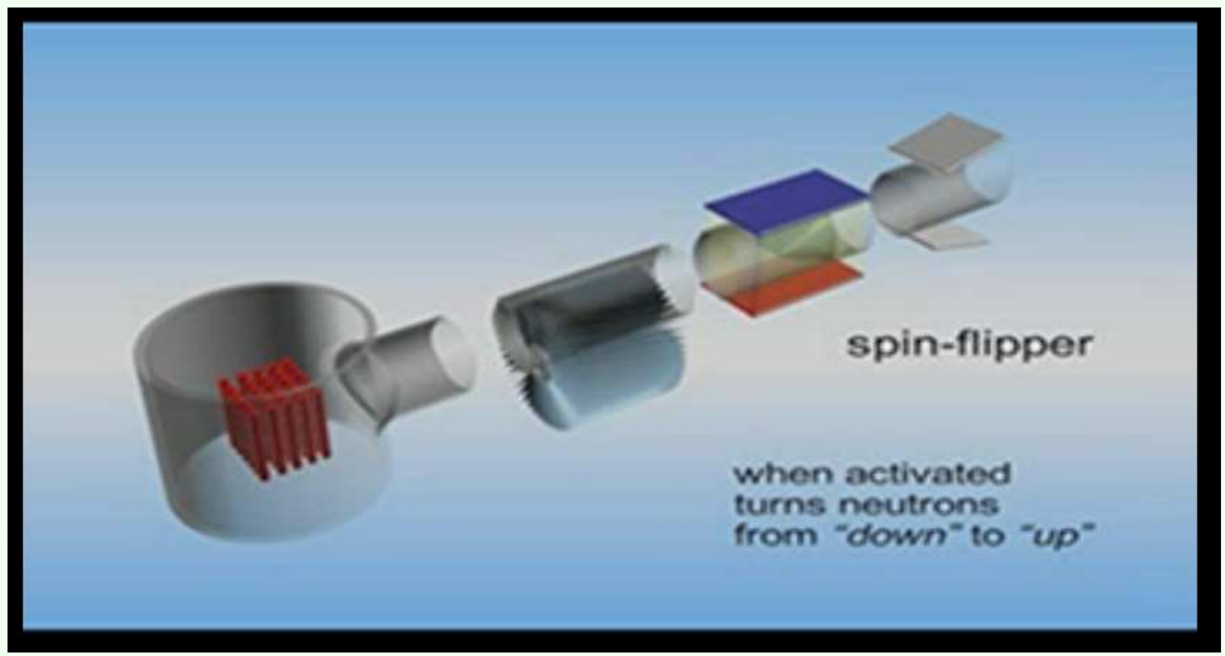


Research areas of interest

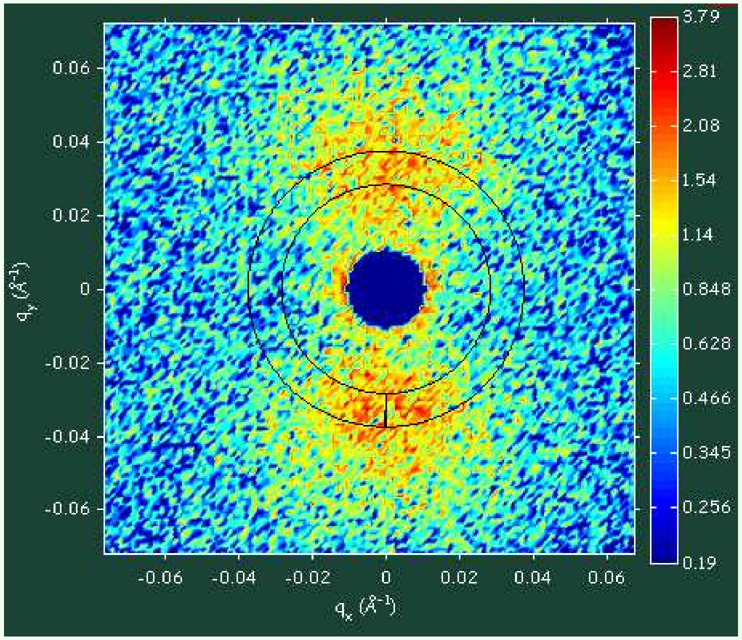




Schematic of a typical SANS instrument

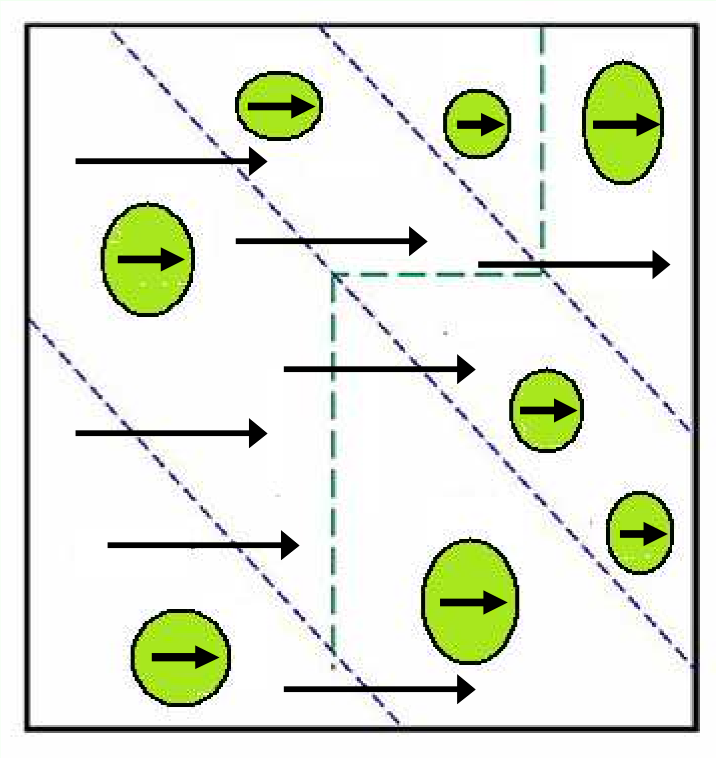


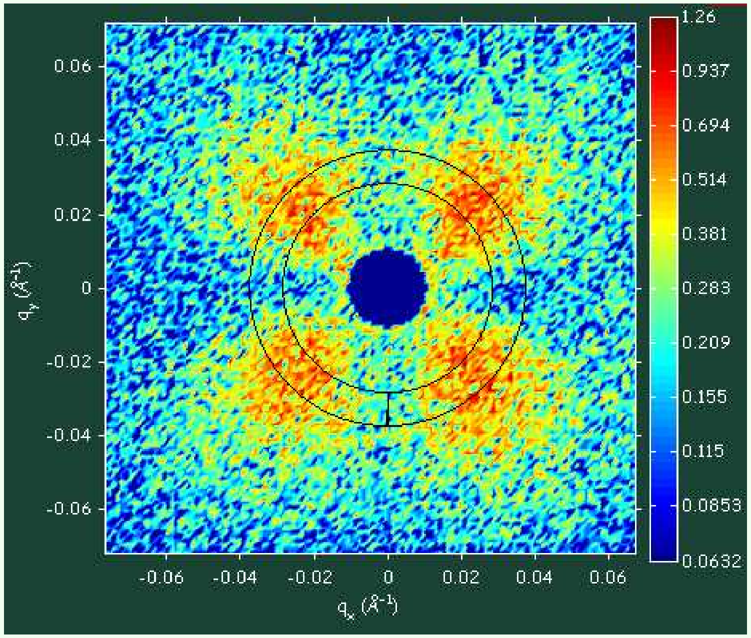
Nuclear or magnetic *scattering* ?



Non-spin flip

H = 13 kG





Spin flip

Results with full polarisation analysis

$$\left[-\frac{\hbar^2}{2m_{\mathrm{n}}}\nabla^2 + V(\mathbf{r})\right]\psi(\mathbf{r}) = E\psi(\mathbf{r})$$

Schrödinger equation

Born approximation – interaction potential *V*(r) treated as a perturbation

OK if scattering is weak, then this is encapsulated by

$$W_{\mathbf{k},\alpha\to\mathbf{k}',\alpha'} = \frac{2\pi}{\hbar}\rho_{\mathbf{k}'}\left|\langle \mathbf{k}'\alpha'|V|\mathbf{k}\alpha\rangle\right|^2 = \frac{2\pi}{\hbar}\rho_{\mathbf{k}'}\left|\int \psi^*_{\mathbf{k}'}\chi^*_{\alpha'}\, V\, \psi_{\mathbf{k}}\chi_\alpha\, \mathrm{d}\mathbf{r}\right|^2$$

Fermi's golden rule

***V*(r) is Fermi pseudo-potential**

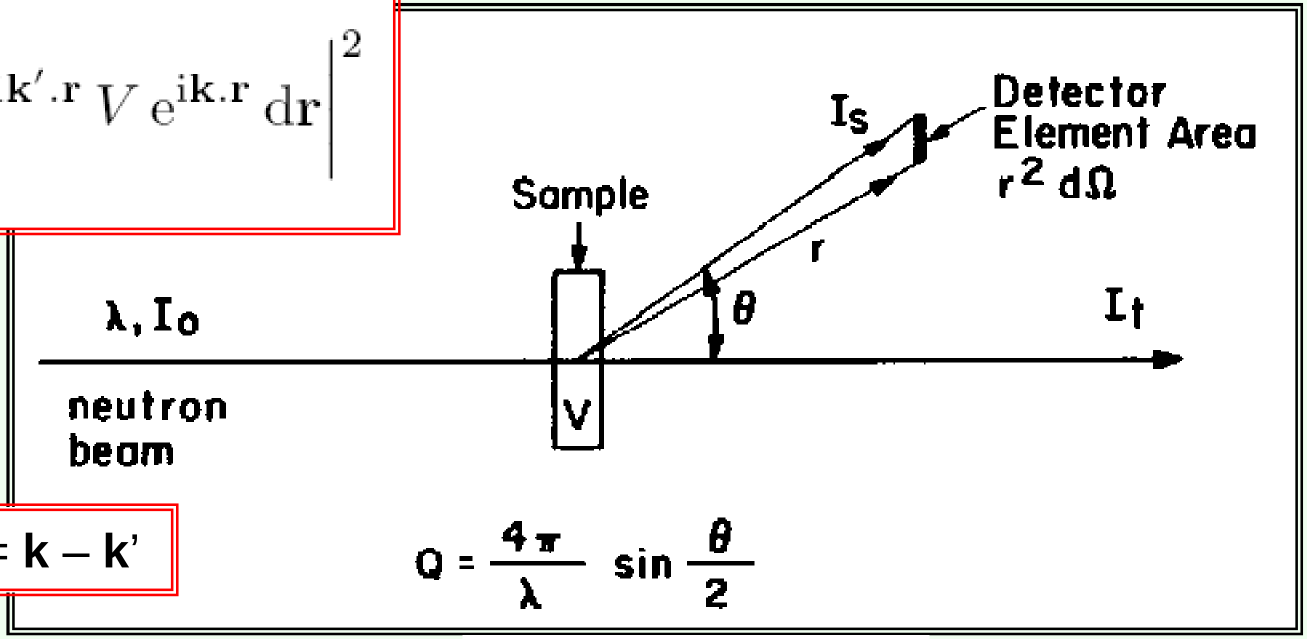
$$\frac{\mathrm{d}\sigma}{\mathrm{d}\Omega} = \frac{1}{\Phi_{\mathrm{n}}}\frac{1}{\mathrm{d}\Omega}\sum_{\mathbf{k}'\in\,\mathrm{d}\Omega} W_{\mathbf{k},\alpha\to\mathbf{k}',\alpha'}$$

Differential cross-section:

probability of neutrons scattering into solid angle dΩ

Revision: non-magnetic scattering

$$\frac{\mathrm{d}\sigma}{\mathrm{d}\Omega} = \left(\frac{m_\mathrm{n}}{2\pi\hbar^2}\right)^2 \left| \int \mathrm{e}^{-\mathrm{i}\mathbf{k}'.\mathbf{r}}\, V\, \mathrm{e}^{\mathrm{i}\mathbf{k}.\mathbf{r}}\, \mathrm{d}\mathbf{r} \right|^2$$



Scattering vector **Q** = ***κ*** = **k** – **k**'

N scatterers each centred at $\mathbf{R}_j$ with same (non-overlapping) potential

$$V = \sum_j^N \hat{V}(\mathbf{r} - \mathbf{R}_j)$$

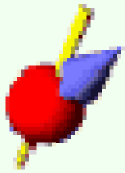
$$\frac{\mathrm{d}\sigma}{\mathrm{d}\Omega} = \left(\frac{m_\mathrm{n}}{2\pi\hbar^2}\right)^2 \left| \int \hat{V}(\mathbf{r})\mathrm{e}^{\mathrm{i}\boldsymbol{\kappa}.\mathbf{r}}\, \mathrm{d}\mathbf{r} \sum_j^N \mathrm{e}^{\mathrm{i}\boldsymbol{\kappa}.\mathbf{R}_\mathrm{j}} \right|^2$$

Form factor $$F_\mathrm{A}(\boldsymbol{\kappa}) \equiv \frac{m_\mathrm{n}}{2\pi\hbar^2} \int \hat{V}(\mathbf{r})\mathrm{e}^{\mathrm{i}\boldsymbol{\kappa}.\mathbf{r}}\, \mathrm{d}\mathbf{r}$$

$$S(\boldsymbol{\kappa}) \equiv \left| \sum_j^N \mathrm{e}^{\mathrm{i}\boldsymbol{\kappa}.\mathbf{R}_\mathrm{j}} \right|^2$$

Structure factor

Revision: non-magnetic scattering



Nuclear magneton

$$\mu_{\mathrm{N}} \equiv \frac{e\hbar}{2m_{\mathrm{p}}}$$

Interaction potential $$-\boldsymbol{\mu}.\mathbf{H} = -\gamma\mu_{\mathrm{N}}\boldsymbol{\sigma}.\mathbf{H}$$

σ is Pauli spin operator

Neutron gyromagnetic ratio

$$\gamma = 1.913$$

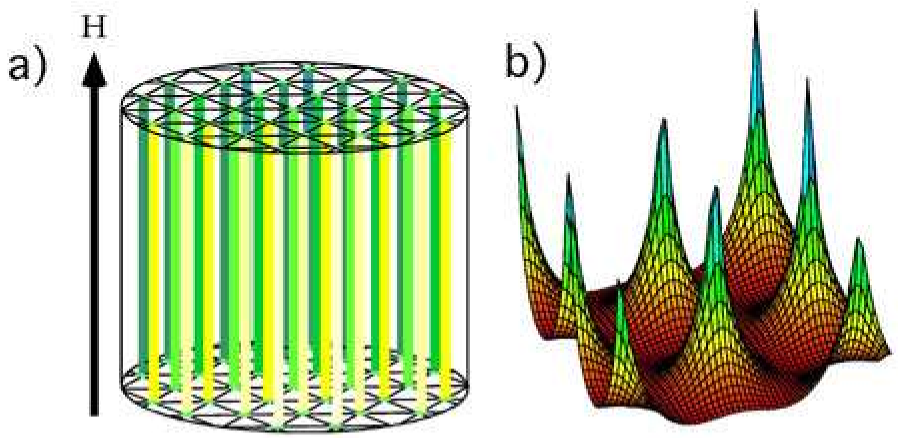
$$\frac{\mathrm{d}\sigma}{\mathrm{d}\Omega} = \left(\frac{m_{\mathrm{n}}}{2\pi\hbar^2}\right)^2 \gamma^2 \mu_{\mathrm{N}}^2 \sum_{\sigma\sigma'} p_\sigma \left|\langle \sigma' \mathbf{k}' | \boldsymbol{\sigma}.\mathbf{H} | \sigma \mathbf{k} \rangle\right|^2$$

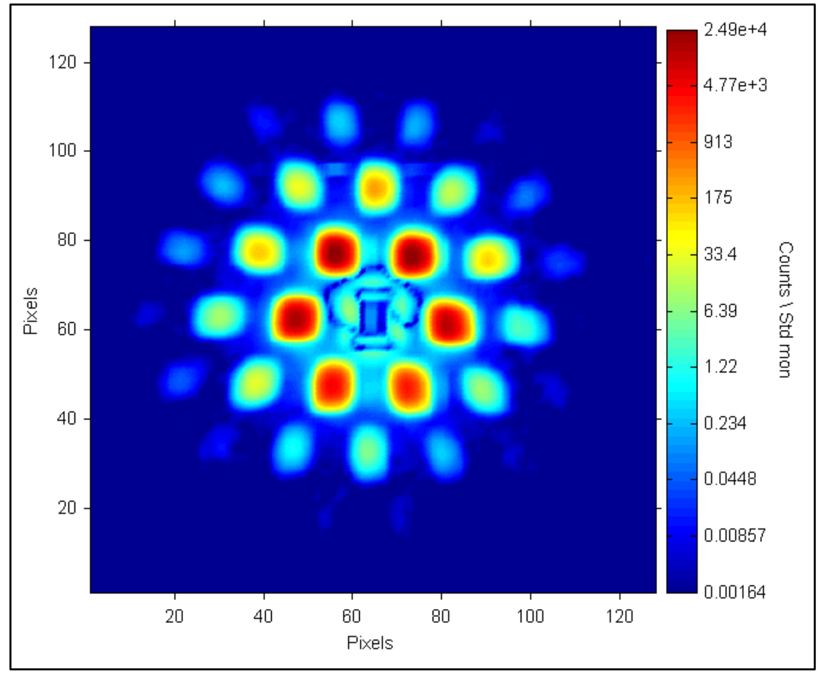
p_σ describes polarisation of incident beam

Simple case !

H is everywhere parallel and unpolarised neutrons $$\mathbf{H} = (0, 0, H)$$

$$\frac{\mathrm{d}\sigma}{\mathrm{d}\Omega} = \left(\frac{m_{\mathrm{n}}}{2\pi\hbar^2}\right)^2 \gamma^2 \mu_{\mathrm{N}}^2 \left| \int H(\mathbf{r}) \mathrm{e}^{\mathrm{i}\boldsymbol{\kappa}.\mathbf{r}} \, \mathrm{d}\mathbf{r} \right|^2 S(\boldsymbol{\kappa})$$





Flux line lattices in (Type-II) superconductors

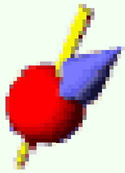
Simple case !

H is everywhere parallel

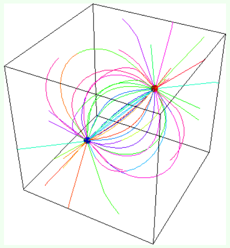
and unpolarised neutrons

$$\mathbf{H} = (0, 0, H)$$

$$\frac{\mathrm{d}\sigma}{\mathrm{d}\Omega} = \left(\frac{m_{\mathrm{n}}}{2\pi\hbar^2}\right)^2 \gamma^2 \mu_{\mathrm{N}}^2 \left| \int H(\mathbf{r}) \mathrm{e}^{\mathrm{i}\boldsymbol{\kappa}.\mathbf{r}} \, \mathrm{d}\mathbf{r} \right|^2 S(\boldsymbol{\kappa})$$



$$\boldsymbol{\sigma}.\mathbf{H} \rightarrow \boldsymbol{\sigma}.\sum_j \mathrm{e}^{\mathrm{i}\boldsymbol{\kappa}.\mathrm{r}_j} \frac{1}{\boldsymbol{\kappa}^2}\left(\boldsymbol{\kappa} \wedge (\mathbf{m}_j \wedge \boldsymbol{\kappa})\right)$$



Halpern-Johnson vector

$$\boxed{\mathbf{Q}_j \equiv \frac{1}{\boldsymbol{\kappa}^2}\left(\boldsymbol{\kappa} \wedge (\mathbf{m}_j \wedge \boldsymbol{\kappa})\right) = \hat{\boldsymbol{\kappa}}(\hat{\boldsymbol{\kappa}}.\mathbf{m}_j) - \mathbf{m}_j}$$

ONLY component of **m** perpendicular to ***κ*** is effective in scattering neutrons

$$\frac{\mathrm{d}\sigma^{\pm\pm}}{\mathrm{d}\Omega}(\mathbf{q}) = \frac{1}{V}\sum_{i,j} \mathrm{e}^{-\mathrm{i}\mathbf{q}.(\mathbf{x}_i - \mathbf{x}_j)}\Big(b_{n,i}b^*_{n,j} \pm b_{n,i}b^*_{m,j}Q^*_{jz}$$

Non Spin-Flip

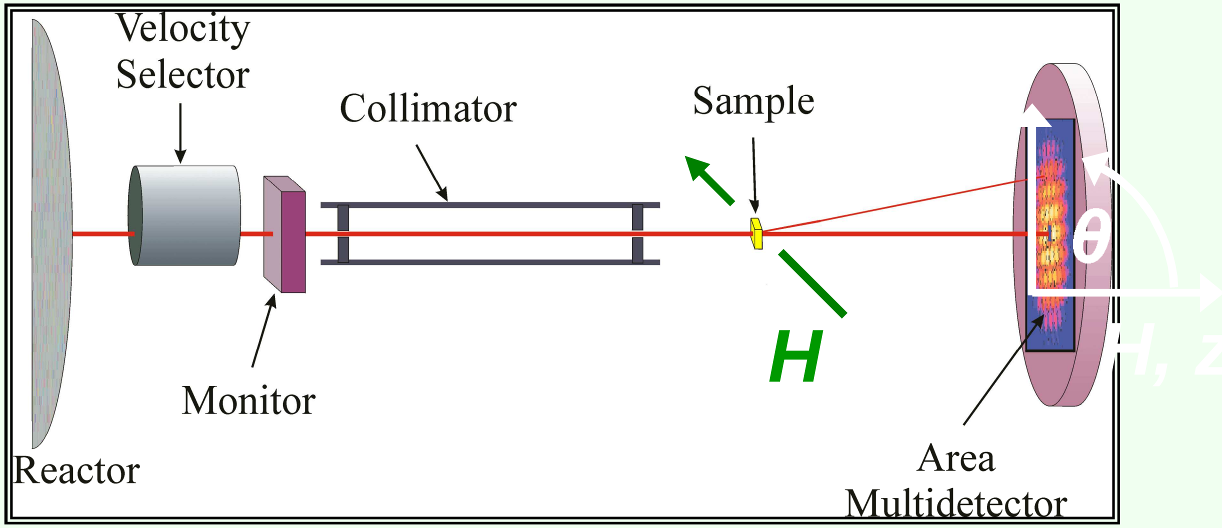
$$\pm b^*_{n,j}b_{m,i}Q_{iz} + b_{m,i}b^*_{m,j}Q_{iz}Q^*_{jz}\Big)$$

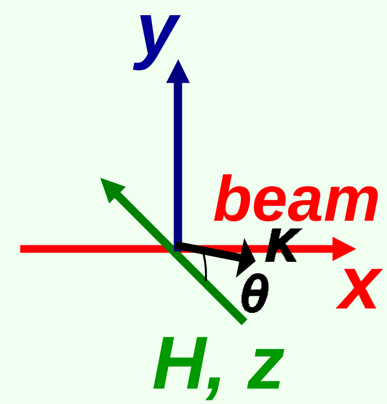
$$\frac{\mathrm{d}\sigma^{\pm\mp}}{\mathrm{d}\Omega}(\mathbf{q}) = \frac{1}{V}\sum_{i,j} \mathrm{e}^{-\mathrm{i}\mathbf{q}.(\mathbf{x}_i - \mathbf{x}_j)} b_{m,i}b^*_{m,j}$$

Spin-Flip

$$\times \left(Q_{ix}Q^*_{jx} + Q_{iy}Q^*_{jy} \mp \mathrm{i}\hat{\mathbf{z}}.(\mathbf{Q}_i \wedge \mathbf{Q}^*_j)\right)$$

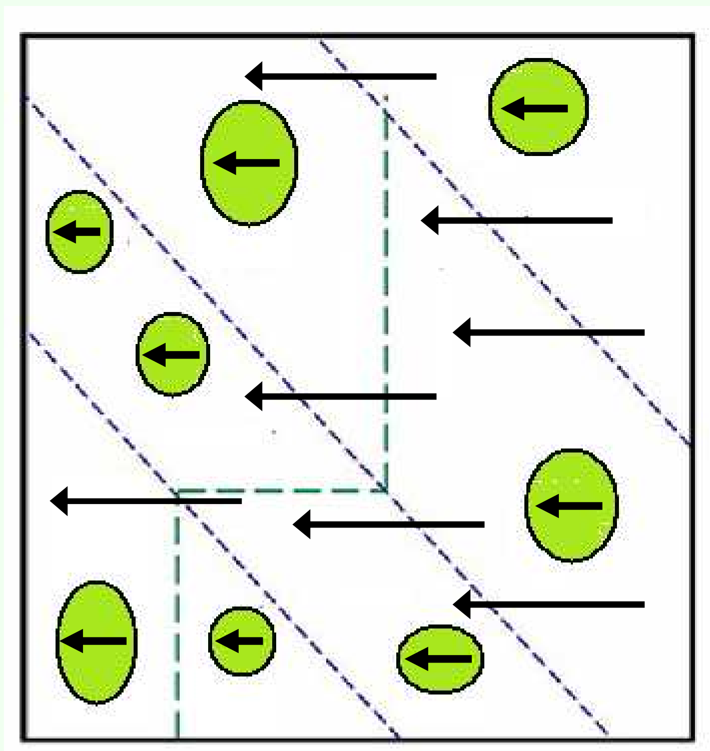
Magnetic scattering from dipole fields





SANS, so

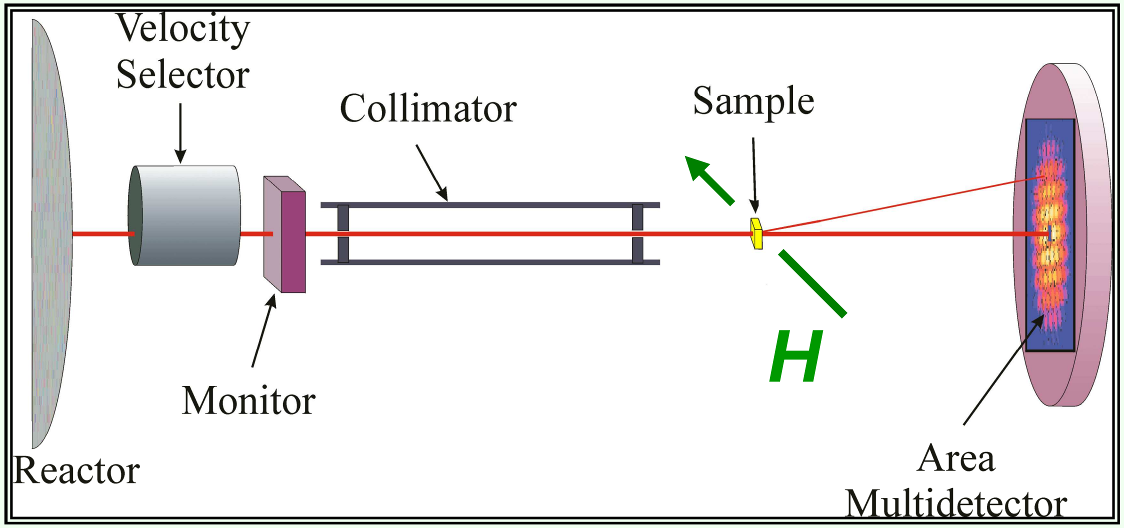
$$\hat{\boldsymbol{\kappa}} = (0, \sin\theta, \cos\theta)$$

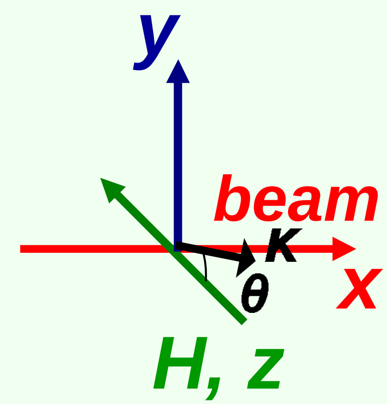


$$\mathbf{m} = (X, Y, Z)$$

$$\mathbf{Q} = \begin{pmatrix} -X \\ -Y\cos^2\theta + Z\sin\theta\cos\theta \\ -Z\sin^2\theta + Y\sin\theta\cos\theta \end{pmatrix}$$

Magnetic, polarised SANS from dipole fields





SANS, so

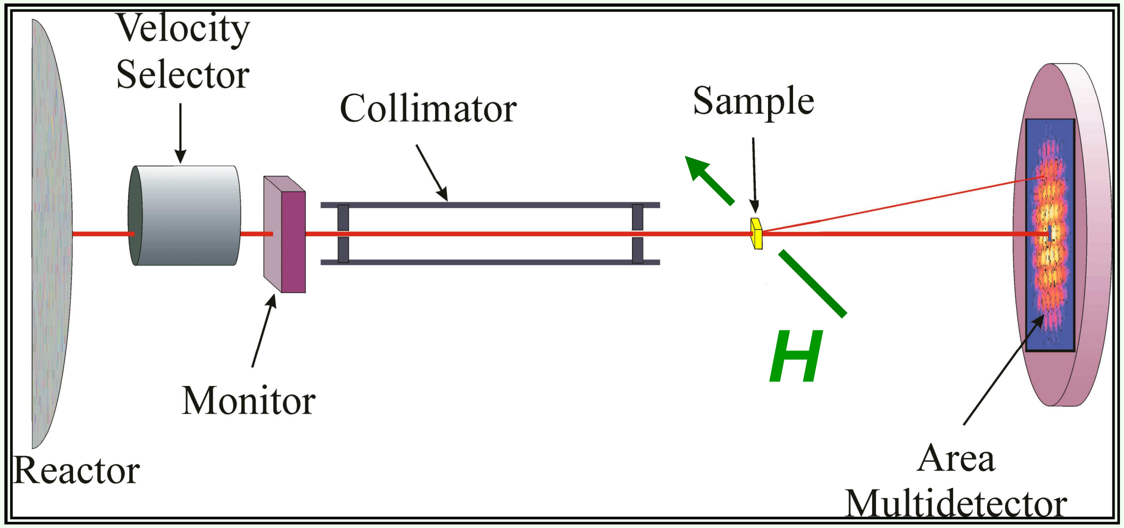
$$\hat{\boldsymbol{\kappa}} = (0, \sin\theta, \cos\theta)$$

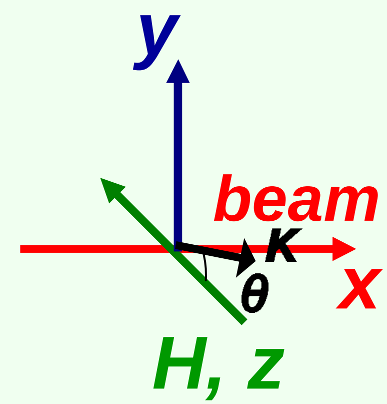
$$\mathbf{m} = (X, Y, Z)$$

$$\begin{aligned}\frac{\mathrm{d}\sigma^{\pm\pm}}{\mathrm{d}\Omega}(\mathbf{q}) \quad = \quad & \frac{1}{V}\sum_{i,j} \mathrm{e}^{-\mathrm{i}\mathbf{q}.(\mathbf{x}_i-\mathbf{x}_j)}\Big(b_{n,i}b^*_{n,j} \mp \big(b_{n,i}b^*_{m,j}Z_j + b^*_{n,j}b_{m,i}Z_i\big)\sin^2\theta \\ & \pm \big(b_{n,i}b^*_{m,j}Y_j + b^*_{n,j}b_{m,i}Y_i\big)\sin\theta\cos\theta \\ & + b_{m,i}b^*_{m,j}\Big(Z_iZ_j\sin^4\theta - (Y_iZ_j + Z_iY_j)\sin^3\theta\cos\theta \\ & + Y_iY_j\sin^2\theta\cos^2\theta\Big)\Big)\end{aligned}$$

Non Spin-Flip

Magnetic, polarised SANS from dipole fields





SANS, so

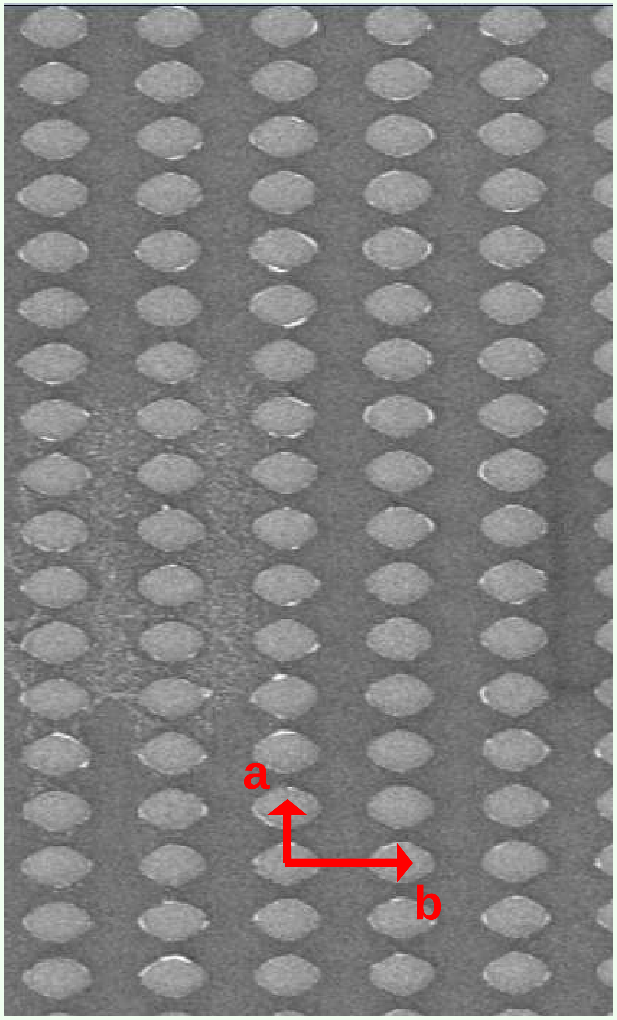
$$\hat{\boldsymbol{\kappa}} = (0, \sin\theta, \cos\theta)$$

$$\mathbf{m} = (X, Y, Z)$$

$$\frac{\mathrm{d}\sigma^{\pm\mp}}{\mathrm{d}\Omega}(\mathbf{q}) = \frac{1}{V}\sum_{i,j} \mathrm{e}^{-\mathrm{i}\mathbf{q}.(\mathbf{x}_i - \mathbf{x}_j)} b_{m,i} b^*_{m,j} \Big(X_i X_j + Y_i Y_j \cos^4\theta - (Y_i Z_j + Z_i Y_j)\sin\theta\cos^3\theta + Z_i Z_j \sin^2\theta\cos^2\theta \Big)$$

Spin-Flip

Magnetic, polarised SANS from dipole fields



$$\mathbf{R}_j = \mu a \hat{\mathbf{x}} + \nu b \hat{\mathbf{y}}$$

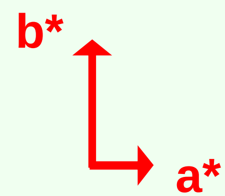
$$S(\boldsymbol{\kappa}) \equiv \left| \sum_j \mathrm{e}^{\mathrm{i}\boldsymbol{\kappa}.\mathbf{R}_j} \right|^2 = \left| \sum_{\mu=0}^{M-1} \mathrm{e}^{\mathrm{i}\mu a \kappa_x} \sum_{\nu=0}^{M-1} \mathrm{e}^{\mathrm{i}\nu b \kappa_y} \right|^2$$

Finite number of particles $N = M^2$

$$S(\boldsymbol{\kappa}) = \frac{\sin^2(a\kappa_x M/2)}{\sin^2(a\kappa_x/2)} \frac{\sin^2(b\kappa_y M/2)}{\sin^2(b\kappa_y/2)}$$

$$\boxed{\boldsymbol{\kappa}_{maxima} = 2\pi \left(\frac{h}{a}, \frac{k}{b} \right) \equiv \mathbf{G}_{hk}}$$

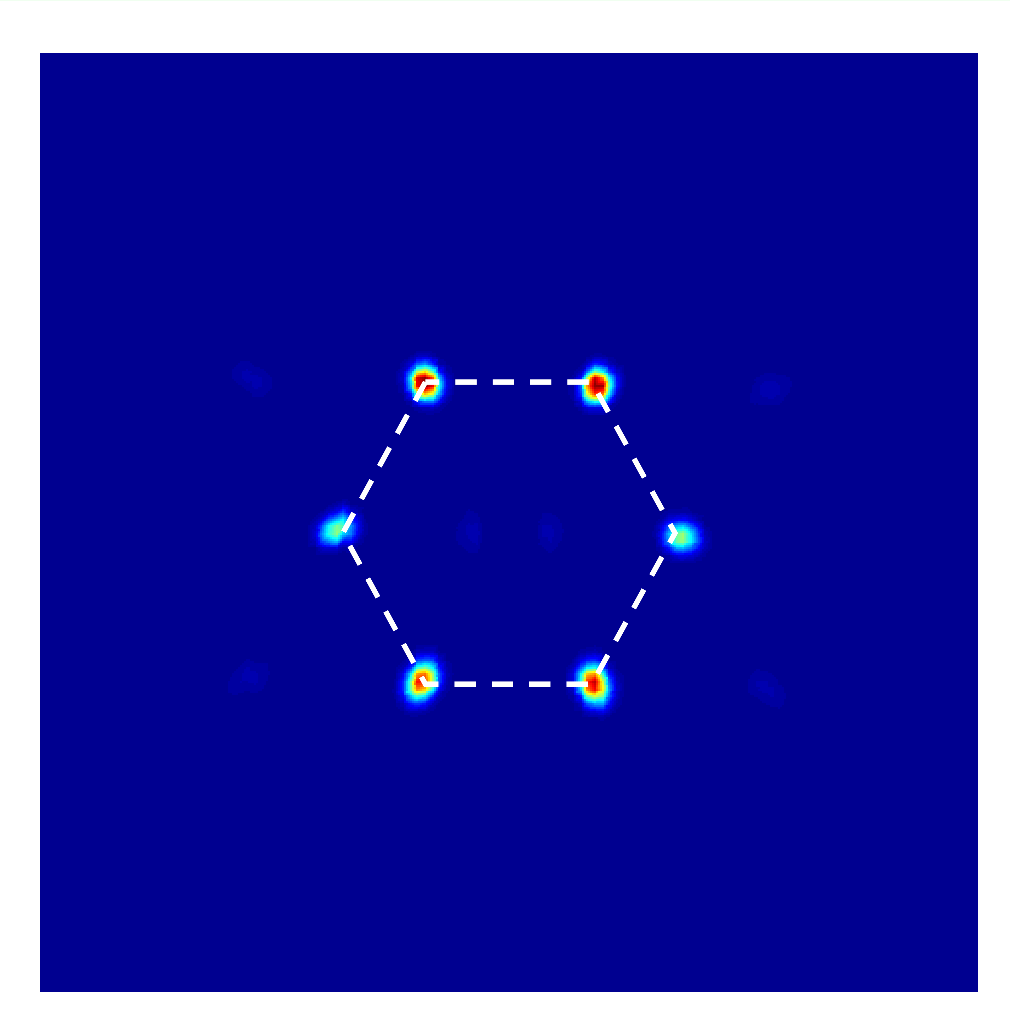
reciprocal lattice vector



Peak width $\sim 1/\sqrt{N}$

$$\boxed{S(\boldsymbol{\kappa}) \to \delta(\boldsymbol{\kappa} - \mathbf{G})}$$

Structure factor

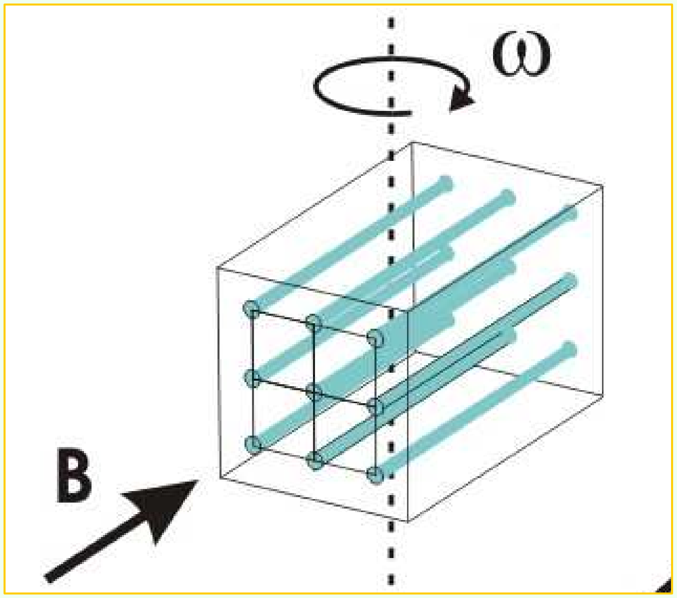


Sum over this rocking curve

$\Phi_0 = B\,A$

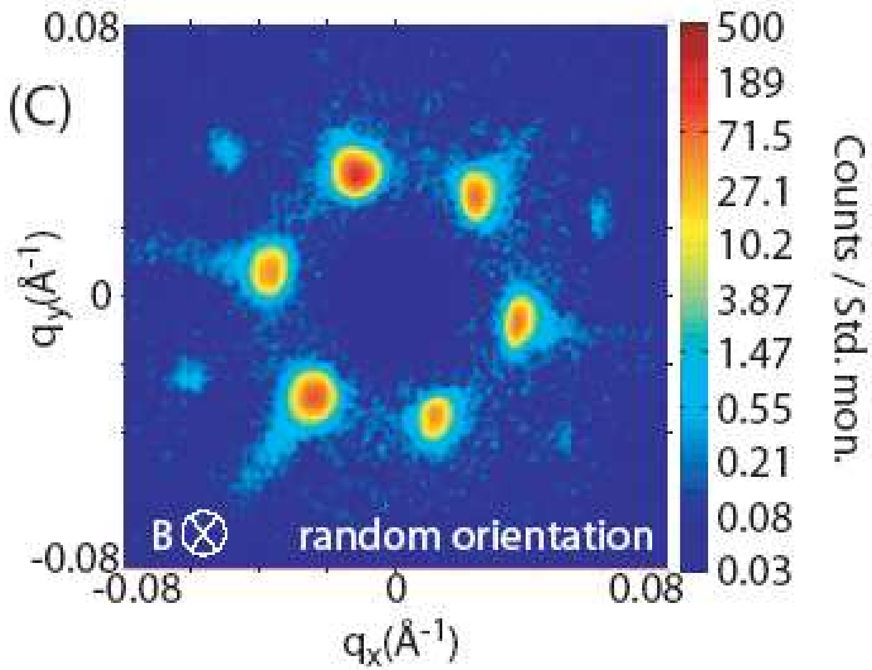
=> $q \sim 0.007$ Å for $B = 200$ mT

=> $\theta \sim 0.3°$ at $\lambda \sim 10$ Å



H || beam

Structure factor – rocking curve

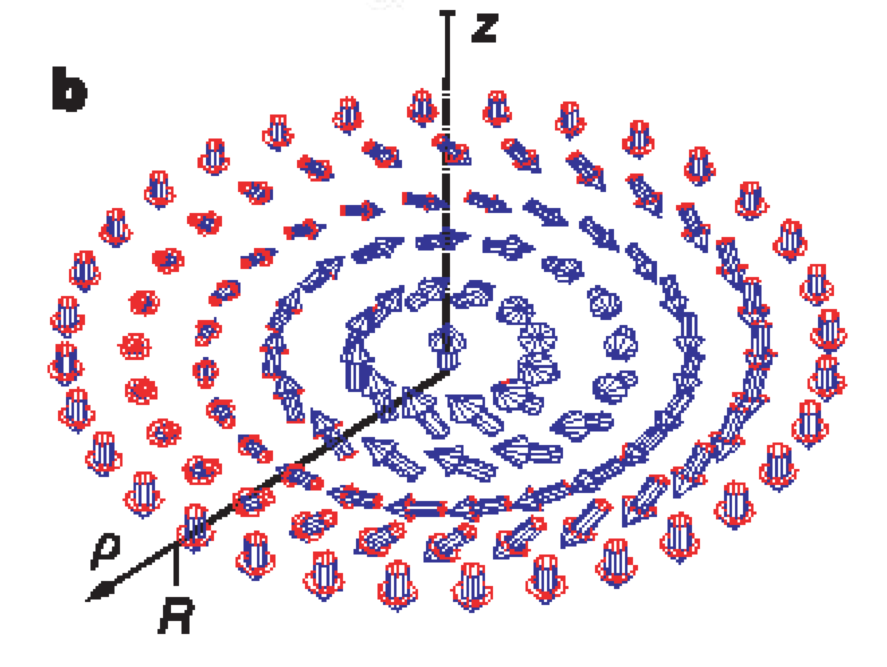


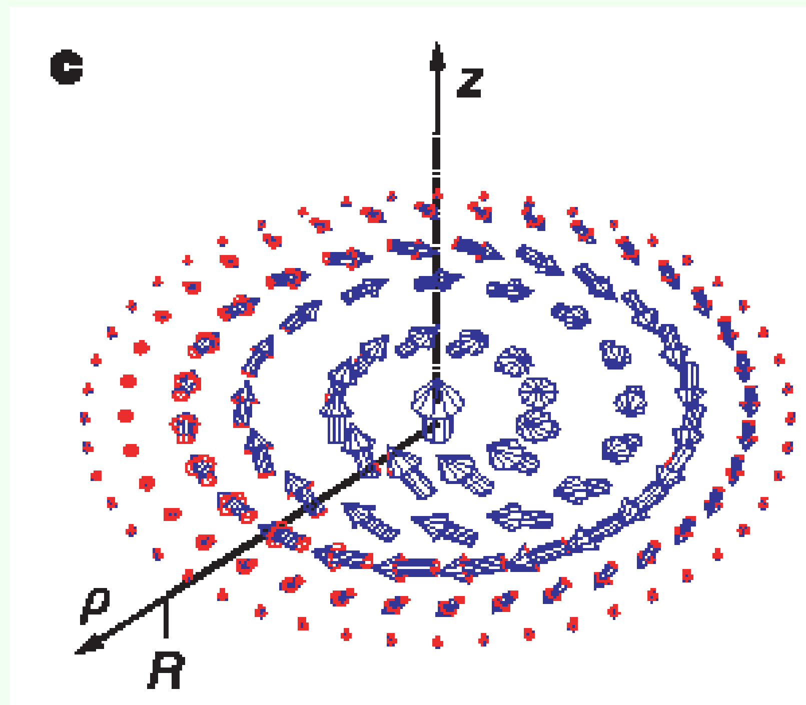
Flux line lattices in superconductors, skyrmion lattices

Magnetic nanoparticles

Films and nano-structured, engineered samples

Phase separated systems, nanocrystalline materials





Typical structure and form factors observed

$$F_N(\boldsymbol{\kappa}) \sim \Delta\eta f(\boldsymbol{\kappa})$$

$$F_M(\boldsymbol{\kappa}) \sim |\Delta\mathbf{Q}|\, f(\boldsymbol{\kappa})$$

$$\Delta\mathbf{Q} \equiv \frac{1}{\boldsymbol{\kappa}^2}\left(\boldsymbol{\kappa} \wedge (\Delta\mathbf{m} \wedge \boldsymbol{\kappa})\right)$$

Nuclear scattering length density

$$N(\boldsymbol{x}) = \sum_{\alpha} b_{\mathrm{n},\alpha}\, \rho_\alpha(\boldsymbol{x})$$

Autocorrelation function

$$C_{\mathrm{N}}(\boldsymbol{r}) = \frac{1}{V}\int \Delta N(\boldsymbol{x})\, \Delta N(\boldsymbol{x}+\boldsymbol{r})\, \mathrm{d}^3x$$

$$\frac{\mathrm{d}\Sigma}{\mathrm{d}\Omega}(q) = \frac{4\pi}{q}\int_0^\infty C_{\mathrm{N}}(r)\, \sin(qr)\, r\, \mathrm{d}r$$

Phase separated systems,
nanocrystalline materials

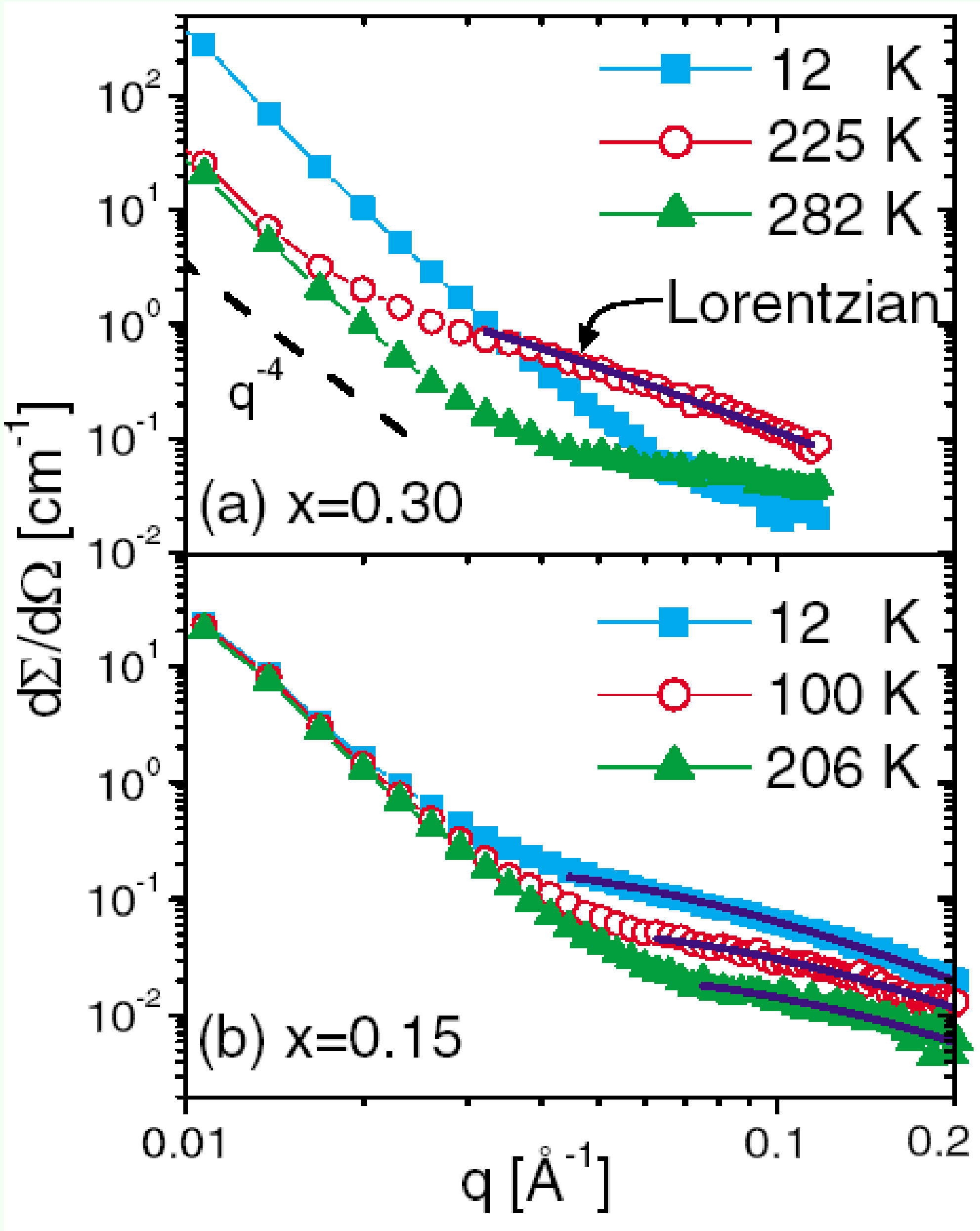
$$C_{\mathrm{N}}(r) = C_0\, \exp(-r\,\kappa)$$

$$\frac{\mathrm{d}\Sigma}{\mathrm{d}\Omega}(q) = \frac{8\pi\, C_0\, \kappa}{(\kappa^2 + q^2)^2}$$

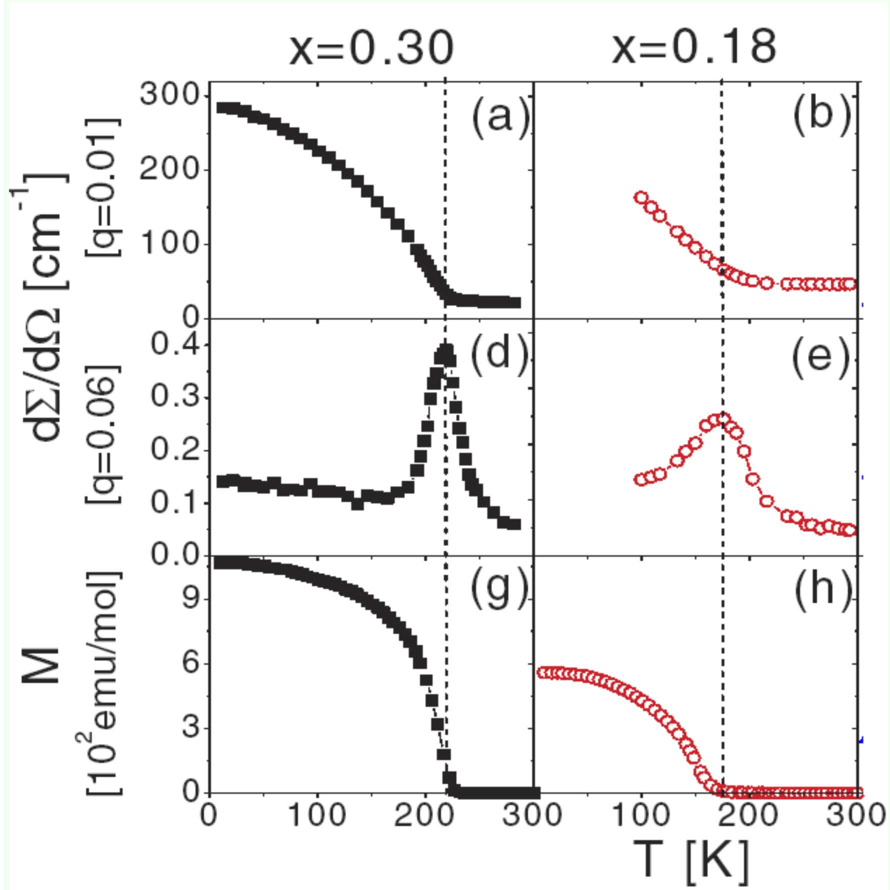
$$C_{\mathrm{N}}(r) = \frac{C_0}{r\,\kappa}\, \exp(-r\,\kappa)$$

$$\frac{\mathrm{d}\Sigma}{\mathrm{d}\Omega}(q) \cong \frac{4\pi\, C_0\, \kappa^{-1}}{\kappa^2 + q^2}$$

Typical structure and form factors observed



Phase separated systems, nanocrystalline materials



$$\frac{d\Sigma}{d\Omega}(q) \cong \frac{4\pi\, C_0\, \kappa^{-1}}{\kappa^2 + q^2}$$

$La_{1-x}Sr_xCoO_3$

Typical structure and form factors observed